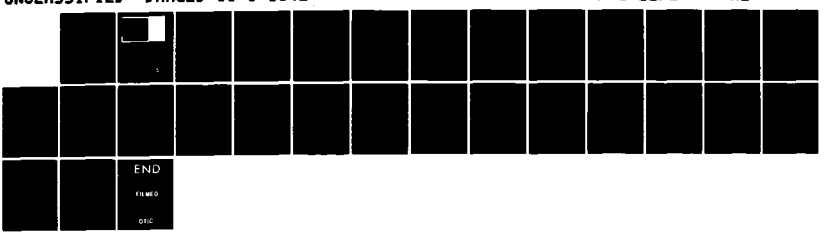
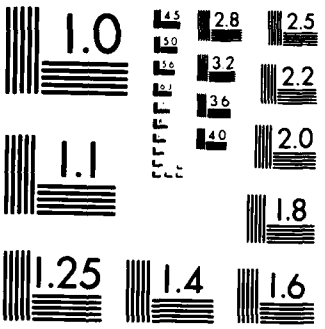
AD-A153 522 LINEAR MODELS FOR FIELD TRIALS SMOOTHING AND CROSS-VALIDATION(U) WISCONSIN UNIV-MADISON MATHEMATICS RESEARCH CENTER P J GREEN 1984 MRC/TSR-2779 1/1

UNCLASSIFIED DAAG29-80-C-0041 F/G 12/1 NL





(2)

AD-A153 522

MRC Technical Summary Report #2779

LINEAR MODELS FOR FIELD TRIALS, SMOOTHING, AND CROSS-VALIDATION

Peter J. Green

Mathematics Research Center
University of Wisconsin—Madison
610 Walnut Street
Madison, Wisconsin 53705

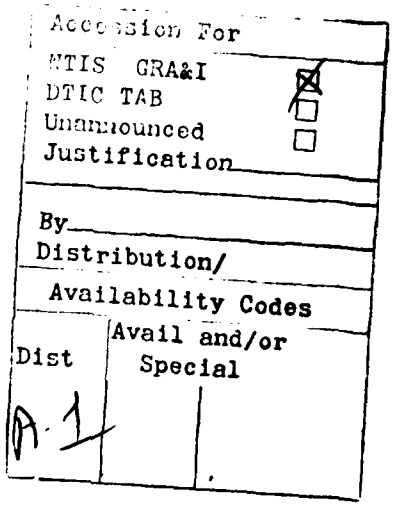
December 1984

(Received November 26, 1984)

Approved for public release
Distribution unlimited

Sponsored by

U. S. Army Research Office
P. O. Box 12211
Research Triangle Park
North Carolina 27709



UNIVERSITY OF WISCONSIN - MADISON
MATHEMATICS RESEARCH CENTER

LINEAR MODELS FOR FIELD TRIALS, SMOOTHING, AND CROSS-VALIDATION

Peter J. Green

Technical Summary Report #2779
December 1984

ABSTRACT

Spatial methods for the analysis of agricultural field experiments are represented here as smoothing methods applied simultaneously with the estimation of treatment effects. Selection of both the form of the smoother and the degree of smoothing required may be based on cross-validation. Particular emphasis is placed in this paper on generalized least-squares estimation in linear models, but the principle applies quite generally.

AMS (MOS) Subject Classifications: 62G05, 62J07, 62P10

Key Words: agricultural field experiments, generalized least-squares, incomplete block designs, neighbour methods, Papadakis method, recovery of inter-block information, smoothing, spatial models.

Work Unit Number 4 - Statistics and Probability

Sponsored by the United States Army under Contract No. DAAG29-80-C-0041.

SIGNIFICANCE AND EXPLANATION

One of the oldest problems in the application of statistics to experimental data is the disentangling of the effects of environmental variation from those of the treatments, whose comparison is the purpose of the experiment. In the context of agricultural field experiments the environmental variation is due to local fluctuations in soil type, nutrient concentrations and micro-climate, summarised by an unknown level of fertility that varies from experimental plot to plot.

Traditionally the statistical analysis of yield data from such experiments has employed block-based methods, which are ideal only under the unrealistic assumption that the fertility level is constant between abrupt breaks at prescribed block boundaries.

Recently there has been much interest in adjusting for fertility in a more continuous manner, recognising that the true fertility profile can probably be more realistically represented as a smooth surface. But the various methods proposed are based on differing statistical principles, so that comparison between methods has been difficult.

The present paper facilitates such comparison by demonstrating that all the techniques suggested, in particular those based on least-squares analysis of a linear model, may be viewed as smoothing methods applied simultaneously with the estimation of additive treatment effects. Comparison of methods reduces to a study of the behaviour and performance of the corresponding smoothers.

It is suggested that cross-validation be used both to choose the degree of smoothing required, and to select the appropriate smoother. Algebraic results are presented that ease the numerical computations involved in this method for a number of important special cases.

LINEAR MODELS FOR FIELD TRIALS, SMOOTHING, AND CROSS-VALIDATION

Peter J. Green

1. Introduction

The aim of many agricultural field experiments is to estimate treatment contrasts efficiently whilst avoiding bias due to trends in fertility and other environmental factors. Blocking methods are customarily used, even when blocks have no physical meaning in the experiment, but there has recently been increasing interest in adjusting for trends in a more continuous way leading to so-called 'spatial' or 'neighbour' methods that deliberately exploit the spatial context.

An early example is the method of adjustment using residuals from neighbouring plots due to Papadakis (1937); see also Bartlett (1978). Succeeding developments have been fostered by increased general interest in spatial methods and by enhanced computing power. Various recent proposals appear in the innovative paper by Wilkinson, Eckert, Hancock and Mayo (1983) and its accompanying stimulating discussion.

The intention of this paper is to increase understanding of the proposed methods, and to aid their comparison, by representing them all as smoothing methods, whether they were originally conceived as such (e.g. Green, Jennison and Seheult, 1983, 1985), or derived from explicit spatial stochastic models (e.g. Besag, 1977), assumed covariance structure (e.g. Williams, 1985b) or other principles (e.g.

Sponsored by the United States Army under Contract No. DAAG29-80-C-0041.

Papadakis; Wilkinson, et al.)

We first demonstrate that the generalized least squares analysis of any linear model is a smoothing method. While this embraces only some of the spatial methods mentioned, it provides an important link with classical block-based analysis. Indeed, for incomplete block designs, Yates's analysis with recovery of inter-block information (1939, 1940) may be regarded as a prototype example for this discussion. The smoothing interpretation extends to analyses not based on least-squares. Later we discuss the choice or estimation of the tuning constant or variance ratio controlling each method, advocating the criterion of cross-validation for this choice; this criterion also provides a means of selecting and assessing the method itself.

Design will not be considered here; no attempt is made at justification or robustification via randomization theory, so design plays no explicit role in analysis. It will of course affect efficiency: for discussion, see Martin (1982) and Williams (1985a).

2. Generalized least squares

Consider the linear model

$$E(y) = D\tau + R\rho; \quad var(y) = \sigma^2 V(\phi) \qquad (2.1)$$

for the vector of yields y from an experiment on n plots to compare a single set of t treatments. Here D is the design matrix for treatment effects τ and R that for any other fixed effects ρ to be fitted; we assume that the complete design matrix $X = [D : R]$ has full rank. The spatial context is represented by appropriate choice of the variance matrix $\sigma^2 V(\phi)$ which is non-singular and

assumed known apart from the multiplier σ^2 and the parameter ϕ, usually scalar.

The presence of ϕ complicates an otherwise trivial estimation problem. If ϕ and hence V are known, generalized least squares leads to the estimating equations

$$X^T V^{-1} \left[y - X \begin{bmatrix} \tau \\ \rho \end{bmatrix} \right] = 0$$

from which ρ may be eliminated to yield the reduced equations for τ alone:

$$D^T (I - S)(y - D\tau) = 0 \qquad (2.2)$$

where (de Hoog, Speed and Williams, 1985)

$$\begin{aligned} S &= I - V^{-1} + V^{-1} R (R^T V^{-1} R)^- R^T V^{-1} \\ &= I - [(I - P_R) V (I - P_R)]^+ \end{aligned} \qquad (2.3)$$

Here I is the $n \times n$ identity matrix, and for any matrix A, A^- denotes any generalized inverse, A^+ the Moore-Penrose inverse, and P_A the projector $A(A^T A)^- A^T$, which is invariant to the choice of generalized inverse. The second form for S emphasizes that not all of V need be specified, only the result after sweeping out the fixed effects in R (see example 2 below).

Since V depends on ϕ, so do S and the generalized least-squares estimate $\hat{\tau}$; these will be denoted $S(\phi)$, $\hat{\tau}(\phi)$ for emphasis where necessary. If the model is correct and ϕ known this is an efficient analysis, and σ^2 may be estimated to quantify the precision of $\hat{\tau}$: however, the least-squares principle does not of itself lead to an estimate of ϕ.

Example 1. Incomplete block designs.

In the analysis of incomplete block designs, with recovery of inter-block information (see Cochran and Cox, 1957, chapters 9 - 11), the assumed variance matrix is $\sigma^2 V(\phi) = \sigma^2(I + \phi P_Z)$; here Z is the design matrix for blocks, so for constant block size k, $P_Z = k^{-1}ZZ^T$. This gives an error structure with two uncorrelated components: plot error with variance σ^2, and random block effects with variance $\sigma^2\phi k^{-1}$. If the design is resolvable, R is taken to be the design matrix for fixed replicate effects; otherwise, R is a single column of 1's to fit an overall mean only. Note that some authors (for example, Nelder (1968)) assume instead that replicate effects are random.

Example 2. Least-squares smoothing.

Green, et al (1983, 1985) describe a method of analysis for field experiments derived from smoothing based on a quadratic penalty function. The version providing one-dimensional adjustment is equivalent to a generalized least squares regression of Δy on ΔD with $\sigma^2(\lambda^{-1}I + \Delta\Delta^T)$ as assumed variance matrix for Δy, where Δ is a rectangular matrix taking second differences along lines of adjacent plots, and λ is a tuning constant. The analysis is invariant to linear trends within lines of adjacent plots, thus we take R to be a design matrix for separate linear regressions in each such line, D fits all treatment contrasts, and V is any matrix such that $\Delta V\Delta^T = \lambda^{-1}I + \Delta\Delta^T$. The tuning constant λ, or λ^{-1}, plays the role of ϕ. This model was also proposed, independently, by Nelder in discussion of Wilkinson, et al (1983).

Other forms of least-squares smoothing are discussed by Green et al. One is equivalent to the linear variance analysis of Patterson (in discussion of Wilkinson, et al (1983)) and Williams (1985b), which uses V as above, but where Δ takes first differences between adjacent plots in the same replicate.

3. The connection with smoothing.

Green, et al (1983) start from an explicit smoothing formulation, and later show its equivalence with generalized least-squares. The connection holds quite generally, and is worth exploiting. It helps to stress that model (2.1) is only assumed in order to generate an analysis, it provides a different interpretation and possible improved algorithms, and it enables us to tie in other methods not equivalent to least-squares for some linear model.

Since $V(\phi)$ is positive definite, we may assume, after possibly re-scaling σ^2 and V, that $V - I$ is non-negative definite. Re-write model (2.1) as

$$y = D\tau + \xi + \eta \qquad (3.1)$$

where $\text{cov}(\xi,\eta) = 0$; $E(\xi) = R\rho$; $\text{var}(\xi) = \sigma^2(V - I)$

$$E(\eta) = 0; \quad \text{var}(\eta) = \sigma^2 I \quad .$$

Now consider the equations:

$$\xi = S(y - D\tau) \qquad (3.2)$$

$$\tau = (D^T D)^{-1} D^T (y - \xi) \quad . \qquad (3.3)$$

Their simultaneous solution gives the generalized least-squares estimate $\hat{\tau}$ (see (2.2)). But if we alternate between (3.2) and (3.3), from any initial estimates, we converge to a minimum of $\Omega(\tau) =$

$(y - D\tau)^T(I - S)(y - D\tau)$ and hence to $\hat{\tau}$. For if (3.2) followed by (3.3) updates τ to τ^*, then $\Omega(\tau^*) = \Omega(\tau) - z^T(I + S)z$ where $z = P_D(I - S)(y - D\tau)$; convergence is obtained if $(I - S)$ is non-negative definite and $(I + S)$ is positive definite, and these are true for S of (2.3). (Further, replacing S by $\alpha S + (1 - \alpha)I$ does not affect the solution to (2.2), so that adjusting α may increase the speed of convergence: it is fastest when $\alpha \approx 2$.)

Generalized least-squares estimates may thus be obtained by alternately performing an ordinary least-squares regression (3.3) on $(y - \xi)$ and smoothing the residuals from fitted treatment effects (3.2). We term S a 'smoother' because its eigenvalues lie in $[0,1]$, with not all of them equal to 0 or 1.

For the example of incomplete block designs, $V = I + \phi P_Z$, $V^{-1} = I - (1 + \phi)^{-1}\phi P_Z$, $P_Z R = R$, so $S = (1 + \phi)^{-1}(P_R + \phi P_Z)$. Thus the relevant 'smoother' involves a weighted average of the block means and the overall mean (or replicate means in the resolvable case). In neighbour methods, S corresponds more closely to the intuitive notion of smoothing.

We should clarify the status of ξ. In the model (3.1) this represents a 'trend' term incorporating both fixed and random effects. Under the additional assumption of joint Normality for ξ and η, the conditional expectation of ξ given y is $(I - V^{-1})(y - D\tau) + V^{-1}R\rho$, whose generalized least-squares estimate $S(y - D\hat{\tau})$ is produced by the alternating iteration described above. This generalizes ridge regression (Hoerl and Kennard, 1970): if τ and ρ are absent, and ξ has prior variance $\sigma^2\lambda^{-1}WW^T$, then

$\xi = W\beta$ where β is estimated by $(W^TW + \lambda I)^{-1}W^Ty$.

When the variance matrix is $\sigma^2V = \sigma^2(I + \Sigma\phi_iW_iW_i^T)$, where $\{\phi_i\}$ and $\{W_i\}$ are known (one or more variance components besides white noise), an alternative representation as a smoothing problem is possible. Taking $\{W_i\}$ to be of full rank, we have implicitly:

$$y = D\tau + R\rho + \Sigma W_i\beta_i + \eta \tag{3.4}$$

where τ and ρ are fixed effects, and $\{\beta_i\}$ and η are uncorrelated zero-expectation random effects with $var(\beta_i) = \phi_i\sigma^2I$ and $var(\eta) = \sigma^2I$. (The identity matrices may be of different orders.) Minimization of the penalty function

$$C = \Sigma\phi_i^{-1}\beta_i^T\beta_i + \eta^T\eta \tag{3.5}$$

subject to the additive model (3.4) leads again to the estimate $\hat{\tau}$. Yet another equivalent formulation is to minimize the ordinary error sum-of-squares $\eta^T\eta$ subject to (3.4) and upper bounds on $\{\beta_i^T\beta_i\}$.

A very similar approach to smoothing is often followed in non-parametric regression problems (Wahba and Wold, 1975; Wahba, 1977). Here the model would be $y_i = \xi(t_i) + \eta_i$ and one possible penalty function is $\int(\xi''(t))^2dt + \Sigma\eta_i^2$.

Natural points of departure for generalizing the least-squares smoother are the simultaneous equations (3.2, 3.3) or the penalty function (3.5). There is no need for S to be symmetric for (3.2) and (3.3) to solve (2.2), so that asymmetric linear estimating equations such as those of Wilkinson et al (1983) may be included. Papadakis's method, whether iterated or not, also fits this formulation naturally. As suggested by Green, et al (1985), alternative robust/resistant analyses may be obtained by use of a non-linear

smoother or treatment estimator in (3.2, 3.3), or by amending the quadratic loss function (3.5).

4. Choosing ϕ

Since ϕ cannot be estimated by least-squares principles, a wide variety of methods for choosing its value have been proposed. Yates's original proposal for incomplete block designs (1939, 1940) entailed equating two suitably chosen sums of squares to expectation, an approach also adopted by Williams (1985b). Alternative estimators for block designs, based on Normal-theory likelihood methods were given by Nelder (1968) and Patterson and Thompson (1971). We return to these criteria in Section 5. For Bayesian viewpoints, see Lindley and Smith (1972) and Box and Tiao (1973, chapter 7).

An attractive, less model-dependent, alternative is to use the criterion of cross-validation, as described by Stone (1974). The idea is to treat each observation in turn as 'missing' and to 'predict' it from the model as fitted to the remaining observations for each given value of ϕ. The parameter ϕ is then chosen to minimize the mean squared error of prediction. Considerable use has been made of cross-validation and related techniques in recent work on smoothing (e.g. Wahba and Wold (1975), Craven and Wahba (1979) and Silverman (1985)). In Stone's terminology, the term 'model' is abandoned as conveying a richer meaning than intended, and replaced by that of a 'prescription' or class of predictors.

Our prescription involves minimizing the weighted sum-of-squares

$$(y - D\tau - R\rho)^T V(\phi)^{-1} (y - D\tau - R\rho)$$

or, equivalently,

$$(y - D\tau)^T(I - S(\phi))(y - D\tau)$$

over choice of τ, ρ (thereby estimating these) and choice of the 'missing' component(s) of y. This is equivalent to fitting a dummy covariate for each missing observation, gives generalized least-squares estimates based on the available data, and provides the conventional 'missing value formula' in the case of uncorrelated data.

Introducing the dummy design matrix E for missing observations gives the augmented model

$$E(y) = D\tau + R\rho + E\gamma, \quad var(y) = \sigma^2 V(\phi) \quad .$$

The reduced estimating equations for the cross-validation errors γ are

$$E^T M(y - E\gamma) = 0$$

where

$$\begin{aligned} M = M(\phi) &= V^{-1} - V^{-1}X(X^TV^{-1}X)^-X^TV^{-1} \\ &= (I - S) - (I - S)D(D^T(I - S)D)^-D^T(I - S) \qquad (4.1) \\ &= [(I - P_{D,R})V(I - P_{D,R})]^+ \quad . \end{aligned}$$

Here, $P_{D,R}$ is the projector for the partitioned matrix $[D \vdots R]$. In particular, if a single observation, y_i say, is deemed to be missing, E consists of a single column of 0's with 1 in row i, and the prediction error $\hat{\gamma} = \hat{\gamma}_{(i)}$, say, is

$$\hat{\gamma}_{(i)} = (E^TME)^{-1}E^TMy = \Big[\sum_{j=1}^{n} M_{ij}y_j\Big] \Big/ M_{ii} \quad .$$

The cross-validation mean squared error is therefore

Silverman, B. W. (1985). Some aspect of the spline smoothing approach to non parametric regression curve fitting (with discussion). J. R. Statist. Soc. B, 47.

Stein, C. (1966). An approach to the recovery of inter-block information in balanced incomplete block designs. Research Papers in Statistics (Neyman Festschrift, F. N. David, ed) 351-366. London: Wiley.

Stone, M. (1974). Cross-validatory choice and assessment of statistical predictions (with discussion). J. R. Statist. Soc. B, 36, 111-147.

Utreras, D., F. (1980). Sur le choix du parametre d'ajustement dans le lissage par fonctions spline. Numer. Math., 34, 15-28.

Utreras, D., F. (1981). Optimal smoothing of noisy data using spline functions. SIAM J. Sci. Stat. Comput., 2, 349-362.

Wahba, G. (1977). A survey of some smoothing problems, and the method of generalized cross-validation for solving them. In Applications of Statistics (P. R. Krishnaiah, ed.), p. 507-523. Amsterdam: North Holland.

Wahba, G. and Wold, S. (1975). A completely automatic French curve: fitting spline functions by cross-validation. Commun. Statist., 4, 1-17.

Wilkinson, G. N., Eckert, S. R., Hancock, T. W. and Mayo, O. (1983). Nearest neighbour (NN) analysis of field experiments (with discussion). J. R. Statist. Soc. B, 45, 151-210.

Wilkinson, J. H. (1965). The Algebraic Eigenvalue Problem. Oxford: Oxford University Press.

de Hoog, F. R., Speed, T. P. and Williams, E. R. (1985). A note on generalized least squares. Submitted to Biometrika.

James, A. T. and Wilkinson, G. N. (1971). Factorization of the residual operator and canonical decomposition of non-orthogonal factors in analysis of variance. Biometrika, 58, 279-294.

Jensen, L. and Stone, M. (1976). Cross-validatory choice of weights for inter- and intra- block estimation in balanced incomplete block designs. Biometrics, 32, 677-681.

John, P. W. M. (1971). Statistical Design and Analysis of Experiments. New York: Macmillan.

Lindley, D. V. and Smith, A. F. M. (1972). Bayes estimates for the linear model. J. R. Statist. Soc. B, 34, 1-41.

Martin, R. J. (1982). Some aspects of experimental design when errors are correlated. Biometrika, 69, 597-612.

Nelder, J. A. (1968). The combination of information in generally balanced designs. J. R. Statist. Soc. B, 30, 303-311.

Papadakis, J. S. (1937). Méthode statistique pour des expériences sur champ. Bull. Inst. Amél. Plantes á Salonique, 23.

Patterson, H. D. and Thompson, R. (1971). Recovery of inter-block information when block sizes are unequal. Biometrika, 58, 545-55'.

Quenou lle, M. H. (1953). The design and analysis of experiments. New York: Macmillan.

Silverman, B. W. (1984). A fast and efficient cross-validation method for smoothing parameter choice in spline regression. J. Am. Statist. Assoc., 79, 584-589.

References

Bartlett, M. S. (1978). Nearest neighbour models in the analysis of field experiments (with discussion) J. R. Statist. Soc. B, 40, 147-174.

Besag, J. E. (1977). Errors-in-variables estimation for Gaussian lattice schemes. J. R. Statist. Soc. B, 39, 73-78.

Box, G. E. P. and Tiao, G. C. (1973). Bayesian inference in statistical analysis. Reading, Mass: Addison-Wesley.

Cochran, W. G. and Cox, G. M. (1957). Experimental designs, 2nd ed. New York: Wiley.

Craven, P. and Wahba, G. (1979). Smoothing noisy data with spline functions: estimating the correct degree of smoothing by the method of generalized cross-validation. Numer. Math, 31, 377-403.

Davies, O. L. (1954). The Design and Analysis of Industrial Experiments. London: Oliver and Boyd.

Green, P. J., Jennison, C. and Seheult, A. H. (1983). Contribution to the Discussion of Wilkinson et. al. (1983), J. R. Statist. Soc. B, 45, 193-195.

Green, P. J., Jennison, C. and Seheult, A. H. (1985). Analysis of field experiments by least squares smoothing. J. R. Statist. Soc. B, 47.

Hoerl, A. E. and Kennard, R. W. (1970). Ridge regression: biased estimation for non-orthogonal problems. Technometrics, 12, 55-67.

Table 3

Simulation for least squares smoothing:

10th and 50th percentiles of percentage efficiency for 5 criteria for choice of ϕ.

Percentile			10th					50th				
Criterion			CV	GCV	Tukey	REML	Lik	CV	GCV	Tukey	REML	Lik
Variance structure	Roughness ϕ_{true}	Design t										
	.02	4	45	47	45	45	45	93	94	94	96	96
		16	79	77	78	80	78	97	97	96	97	97
	.2	4	38	37	36	35	36	88	84	87	89	89
		16	73	73	76	78	76	95	94	93	93	93
	.02	4	40	39	36	37	39	87	85	84	88	86
		16	71	65	75	78	74	95	95	95	96	96
	.2	4	18	17	19	17	19	79	81	79	78	77
		16	70	71	74	71	67	92	92	94	93	93
	.02	4	42	42	42	42	42	94	93	96	96	96
		16	77	80	82	85	82	97	97	98	98	97
	.2	4	25	27	28	26	26	83	84	89	84	87
		16	71	71	71	75	70	88	90	90	93	90

Designs (each 48 plots in one line)

t=4)

2 3 2 1 4 3 4 1 2 1 3 4 2 1 2 3 4 3 2 4 1 4 1 3 2 3 1 2 4 2 4 3 1 3 1 4 2
2 1 4 3 4 1 2 1 3

(t=16)

4 16 12 7 11 3 15 1 13 5 9 6 2 10 14 5 12 15 2 3 14 8 9 11 16 6 1 7 10 4
3 11 2 13 8 6 4 15 9 16 5 3 10 7 12 14 1

examine the criteria marginally: an appropriate measure of the efficiency of a particular choice ϕ^* is

$$\frac{\min_{\phi} \sum_{j=1}^{t} (\hat{\tau}_j(\phi)-\tau_j)^2}{\sum_{j=1}^{t} (\hat{\tau}_j(\phi^*)-\tau_j)^2}$$

where $\{\tau_j\}$ are the true values, here zero. Note that 100% efficiency cannot be attained. For each criterion, the empirical distribution of efficiency, from the 100 replicates, was constructed. Some of the results are presented in Table 3. They demonstrate rather close agreement between the criteria, and suggest no clear preferences. The superiority of generalized cross-validation over the ordinary version found by Craven and Wahba (1979) is not apparent here, presumably because of the well-conditioned nature of these designed experiments.

Since the other criteria are less readily adapted to a variety of smoothing methods, especially those not derived from least-squares, these results support the use of cross-validation for choice of ϕ.

Acknowledgements.

I am particularly grateful to Robin Thompson for making the connection with restricted maximum likelihood, to Chris Jennison for other constructive comments on an earlier version of this paper, and to the referees for suggestions that greatly simplified the algebraic details.

algebraic results in Sections 4, 5 and 6. The form of $V(\phi)$ assumed was that corresponding to ordinary least-squares smoothing (example 2 in Section 2). Three factors were varied in the experiment.

(I) The true variance structure for y: three alternatives, in each case white noise η plus correlated ξ, all jointly Normally distributed with (a) first differences or (b) second differences of ξ independent and identically distributed, or (c) ξ as a 7-point equally weighted moving average.

(II) The true roughness, measured by $\phi_{true} = (n\xi^T\Delta^T\Delta\xi)/\{(n-2)\eta^T\eta\}$: two alternatives, .02 and .2.

(III) The design (and number of treatments): two alternatives, both with $n = 48$ plots: one adapted from a serially balanced design on 4 treatments, the other a triple lattice with 3 replicates of 16 treatments, block size 4.

For each of the resulting $12 = 3 \times 2 \times 2$ cases, 100 replicates were performed: ξ and η were drawn independently from (I) and scaled according to (II), then the sum $y = \xi + \eta$ analysed by least-squares smoothing assuming design (III). Thus true treatment effects were set to zero.

Five criteria were compared: ordinary and generalized cross-validation, and three methods suggested in Green, Jennison and Seheult (1985): 'Tukey's rule', in which $y^TMy/(tr(M))^2$ is minimized, and full and restricted maximum likelihood. The resulting choices of ϕ were extremely highly correlated. It was therefore sufficient to

Table 2

Choice of ϕ in second-difference least-squares smoothing: data-sets as described and analysed in Green, et al (1985).

	Data Set		
	Mildew	SB 77 ES 5	SB 77 ES 6
n,t	38,4	51,17	48,16
Estimate			
Yates	0.11	0.0162	0.0603
Tukey	1.86	0	0.0613
Restricted maximum likelihood	2.79	0.0041	0.0591
Generalized cross-validation	3.06	0.0051	0.0809
Cross-validation	3.40	0.0022	0.1113
Maximum likelihood	5.27	0.0238	0.1915

6. Application to least-squares smoothing

The spectral decomposition of M given in (5.1) reduces the computation in least-squares smoothing methods, whether in the form based on second differences as discussed in detail by Green, et al (1985) or in the generalizations described here.

All of the methods for choosing the tuning constant ϕ^{-1} proposed by Green, et al involve computing the decomposition $y = D\hat{\tau} + \hat{\xi} + \hat{\eta}$ for several values of ϕ^{-1}. The spectral decomposition (5.1), while incurring a set-up cost, permits the decomposition and various derived statistics to be computed very cheaply for subsequent values of ϕ^{-1}.

When $V(\phi) = I + \phi WW^T$, note that $V^{-1} = I - W(\phi^{-1} I + W^TW)^{-1}W^T \to I - P_W$ as $\phi \to \infty$. The fixed effects τ, ρ in model (2.1) are estimated by Ty where $T = T(\phi) = (X^TV^{-1}X)^{-1}X^TV^{-1}$. Note that $M = V^{-1}(I-XT)$. Now

$$T(\infty)\ (I-M(\phi)) = (X^T(I-P_W)X)^{-1}X^T(I-P_W)(I-V(\phi)^{-1}(I-XT(\phi))) = T(\phi)$$

since $(I-P_W)(I-V^{-1}) = 0$. Thus if we write $\hat{\eta} = \hat{\eta}(\phi) = M(\phi)y$, the decomposition of $y-\hat{\eta}(\phi)$ as $D\hat{\tau}(\phi) + \hat{\xi}(\phi)$ is obtained by linear transformations not depending on ϕ: only $M(\phi)$ need be re-computed for each ϕ, and that from the spectral decomposition (5.1).

Numerical examples of choices of ϕ are given in Table 2: the data-sets are those used by Green, et al (1985).

7. A simulation study

To compare the use of cross-validation in choosing ϕ with other criteria, we performed a simulation experiment, making use of the

To derive an analogue of Yates' estimate for ϕ valid for general known W in $V = I + \phi WW^T$, note that in consequence of (5.1) S_X and $S_{X,W}$ are the limits, as $\phi \to 0$ and ∞ respectively, of the weighted error sum-of-squares $\Gamma(\phi) = y^T My = \min_{\tau,\rho}\{(y-D\tau-R\rho)^T V^{-1}(y-D\tau-R\rho)\}$ that would be the focus of attention if ϕ were <u>known</u>. Equating $\Gamma(0)$ and $\lim_{\phi\to\infty}\Gamma(\phi)$ to expectation under model (2.1) therefore seems the natural analogue, although this procedure is not as cheap and convenient as in the incomplete blocks case, because the expectations in general involve non-trivial trace terms. Further, if D, R and W together span $\mathbf{R}^n$, e.g. least-squares smoothing with first or second differences, $\Gamma(\phi) \to 0$ as $\phi \to \infty$. In this situation, Williams (1985b) tacitly uses $\lim_{\phi\to\infty} \phi\Gamma(\phi)$ as the second sum of squares: from (5.1) we see that this equals $y^T Ny$, where $N = [(I - P_X)WW^T(I - P_X)]^+$. Provided that $(I - P_V)(I - P_R) = 0$, the result of de Hoog, <u>et al</u> (1985) stated in (2.4) remains true when V is singular, if V^{-1} is replaced by V^+. Thus, replacing V by WW^T and R by X, we see that if $(I - P_W)(I - P_X) = 0$ we have

$$N = \Delta^T\Delta - \Delta^T\Delta X(X^T\Delta^T\Delta X)^- X^T\Delta^T\Delta$$

$$= \Delta^T(I - P_{\Delta X})\Delta$$

if Δ is chosen so that $(WW^T)^+ = \Delta^T\Delta$; for example $\Delta = (W^TW)^{-1}W^T$ if W has full rank. Thus y^TNy is the residual sum-of-squares from ordinary regression of Δy on ΔX.

Table 1

Balanced incomplete block designs:

estimate of ϕ for four data sets, according to five different criteria.

	Data set				
	Davies (1954, p207)	Davies (1954, p216)	Quenouille (1953, p177)	John (1971, p226)	Ditto, fitting replicates
n,t,k	12,4,3	20,5,4	30,6,3	36,9,3	36,9,3
Estimate					
Jensen and Stone (1976)*	13.08	-0.6357	2.938	-0.4444	-
Yates (1940)	21.40	-0.5033	3.320	0.1348	-0.1685
Cross-validation as described here	21.40	-0.5033	3.446	0.1975	-0.1685
Nelder (1968)	21.40	-0.5033	3.355	0.2102	-0.1685
Stein (1966)*	68.32	0.2640	9.123	0.4303	-

Notes: Where ϕ is estimated as negative, it would be customary to use $\phi = 0$, i.e. to use no block adjustment. The rows marked * were given for these data sets by Jensen and Stone. Nelder's estimates are identical with those of Patterson and Thompson (1971) since the blocks are of equal size.

squares, $y^T(I - P_{X,W})y = S_{X,W}$, and the blocks sum-of-squares, within replicates if relevant, adjusted for treatments, $y^T(P_{X,W} - P_X)y = S_X - S_{X,W}$.

The requirement of equality of the non-zero eigenvalues $\{\lambda_j\}$ is strong. It demands considerable implicit symmetry in the design; for example, it does not apply to all balanced incomplete blocks designs. If WW^T is proportional to a projector for some factor, the requirement is of first-order-balance for this factor with respect to X, in the sense of James and Wilkinson (1971).

Some numerical examples are given in Table 1 for the same collection of BIBD's considered by Jensen and Stone (1976) in their application of cross-validation to these designs. Note the exact or close agreement between cross-validation and the criteria of Yates (1940), Nelder (1968) and Patterson and Thompson (1971). When the eigenvalues $\{\lambda_j\}$ differ, the exact connection is broken; however if they do not differ too markedly, the argument above suggests approximate equivalence of the two criteria.

It will be noted from Table 1 that Jensen and Stone (1976) obtained different weights from a cross-validation argument based on a different prescription. They obtain separate predictors for the intra- and inter-block extremes of $\phi(\infty$ and $-1)$ regarding an entire block as missing in deriving the inter-block predictor. The Stein estimates differ considerably from the rest, apparently because they utilize inter-block information only through the treatment component: Stein's estimator (1966) uses only $\hat{\tau}(-1)$, $\hat{\tau}(\infty)$ and $S_{X,W}$.

Since the two terms are symmetric and commute, they may be simultaneously diagonalized (Wilkinson, 1965, p. 52) and then using the idempotence of $I - P_X$ it is straightforward to prove the existence of an orthogonal matrix U partitioned as $[U_1\ U_2\ U_3]$, where U_i has r_i columns, and a diagonal matrix Λ of positive eigenvalues $\{\lambda_j\}$ such that $P_X = U_1U_1^T$, $(I - P_X)WW^T(I - P_X) = U_2\ \Lambda\ U_2^T$ and $I - P_{X,W} = U_3U_3^T$. Then

$$M(\phi) = U_2(I + \phi\Lambda)^{-1}U_2^T + U_3U_3^T \qquad (5.1)$$

so that M has eigenvalues 0 and 1 with multiplicities r_1 and r_3, and also $\{(1 + \phi\lambda_j)^{-1},\ j = 1,2,\ldots,r_2\}$. Note that this explicitly demonstrates how M varies from $(I - P_X)$ to $(I - P_{X,W})$ as ϕ increases from 0 to ∞; for example, in the incomplete blocks model these limits corresponding to ignoring block effects, and to fitting them as fixed, respectively. The decomposition used here is essentially that used by Patterson and Thompson (1971) for block models.

It follows from (5.1) that $(d/d\phi)M = \phi^{-1}(M^2 - M)$, so that by the remarks at the end of the previous section, generalized cross-validation is equivalent to equating to expectation y^TM^ry for $r = 2$ and 3, and restricted maximum likelihood similarly for $r = 1$ and 2.

When the $\{\lambda_j\}$ are equal, all positive powers of M are convex combinations of $I - P_X$ and $I - P_{X,W}$ so that <u>both</u> criteria are algebraically equivalent to Yates's estimate of ϕ for incomplete block designs (1939, 1940); in our notation, with $W = P_Z$, this entails equating to expectation the intra-block residual sum-of-

structure $V(\phi)$, presumably in practice from a small number of alternatives. Coupled with cross-validatory assessment of that choice (Stone, 1974), this may be the only reasonable way to choose between methods on the basis of an individual data set, rather than, for example, from uniformity data believed to have similar covariance structure.

Mr. Robin Thompson has pointed out to me an interesting parallel between the present approach and that of restricted maximum likelihood, which may be stated in some generality as follows. Differentiating (4.3) with respect to ϕ and noting that $MX = 0$ and $MVM = M$ reveals that generalized cross-validation is equivalent to equating to their expectation under (2.1) certain sums-of-squares, namely $y^T M^2 y$ and its derivative, or for vector ϕ all partial derivatives. The restricted maximum likelihood approach of Patterson and Thompson (1971), generalized to arbitrary V, does the same but with M^2 replaced by M. Some numerical comparisons will be made in Section 5 and 6.

5. A spectral decomposition

We now restrict attention to variance structures of the form $V = I + \phi WW^T$ for some known matrix W, representing plot error with one other variance component: ϕ is the ratio of variances. This includes the incomplete blocks model, and least-squares smoothing based on first or second differences.

From (4.1) we have

$$M^+ = (I - P_X)V(I - P_X) = (I - P_X) + \phi(I - P_X)WW^T(I - P_X) \quad .$$

$$C(\phi) = n^{-1} \sum_{i=1}^{n} \hat{\gamma}_{(i)}^{2} = \frac{1}{n} \sum_{i=1}^{n} \left[\left[\sum_{j=1}^{n} M_{ij} y_j \right] \Big/ M_{ii} \right]^2 \quad . \qquad (4.2)$$

Thus, by analogy with Wahba (1977) and Craven and Wahba (1979), there is an algebraic form for $C(\phi)$ that can be computed without performing n separate regression calculations. However, there is still usually a much greater burden in evaluating $M(\phi)$ than in finding $\hat{\tau}(\phi)$. Some short-cuts are possible (see Sections 5 and 6; also Craven and Wahba (1979)), but to alleviate the problem, and to acquire a form of rotation-invariance, Wahba (1977) proposed an alternative criterion of <u>generalized cross-validation</u>, derived by replacing M_{ii} in (4.2) by its average, $n^{-1}\mathrm{tr}(M)$, to give

$$G(\phi) = n(\mathrm{tr}(M))^{-2} \, y^T M^2 y \quad . \qquad (4.3)$$

Under certain conditions of balance or symmetry in designed experiments, the M_{ii} are equal. Choice of ϕ, whether scalar or vector-valued, can be made in practice by numerical minimization of (4.2) or (4.3): for scalar ϕ, we have found that both golden-section and quadratic interpolation on $\log \phi$ work well.

In the context of non-parametric regression, Silverman (1984) uses results of Utreras (1980, 1981) to amend the criterion further, by calculating the trace from eigenvalue approximations.

When using a smoother S not of the form (2.3), these algebraic simplifications are not available, but the principle of cross-validation may still be used. The prescription must define how to smooth across the gap caused by a missing observation.

A logical extension to cross-validation for selecting the parameter ϕ is to allow it to choose the form of the variance

Williams, E. R. (1985a). A criterion for the construction of optimal neighbour designs. To appear in J. R. Statist. Soc. B.

Williams, E. R. (1985b). A neighbour model for field experiments. Submitted to Biometrika.

Yates, F. (1939). The recovery of inter-block information in variety trials arranged in three-dimensional lattices. Ann. Eugen., 9, 136-156.

Yates, F. (1940). The recovery of inter-block information in balanced incomplete block designs. Ann. Eugen., 10, 317-325.

PJG/jvs

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER #2779	2. GOVT ACCESSION NO. AD-A153522	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Linear Models for Field Trials, Smoothing, and Cross-Validation		5. TYPE OF REPORT & PERIOD COVERED Summary Report - no specific reporting period 6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Peter J. Green		8. CONTRACT OR GRANT NUMBER(s) DAAG29-80-C-0041
9. PERFORMING ORGANIZATION NAME AND ADDRESS Mathematics Research Center, University of Wisconsin 610 Walnut Street Madison, Wisconsin 53706		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS Work Unit Number 4 - Statistics and Probability
11. CONTROLLING OFFICE NAME AND ADDRESS U. S. Army Research Office P.O. Box 12211 Research Triangle Park, North Carolina 27709		12. REPORT DATE December 1984 13. NUMBER OF PAGES 24
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)		15. SECURITY CLASS. (of this report) UNCLASSIFIED 15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

agricultural field experiments, generalized least-squares, incomplete block designs, neighbour methods, Papadakis method, recovery of inter-block information, smoothing, spatial models.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Spatial methods for the analysis of agricultural field experiments are represented here as smoothing methods applied simultaneously with the estimation of treatment effects. Selection of both the form of the smoother and the degree of smoothing required may be based on cross-validation. Particular emphasis is placed in this paper on generalized least-squares estimation in linear models, but the principle applies quite generally.

DD FORM 1 JAN 73 1473 EDITION OF 1 NOV 65 IS OBSOLETE

UNCLASSIFIED

SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

END

FILMED

6-85

DTIC